

APPROXIMATION FOR A TOY DEFECTIVE ISING MODEL

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Abstract

It has been previously shown that one can use the ME methodology (Caticha Giffin 2006) to reproduce a mean field solution for a simple fluid (Tseng 2004). One could easily use the case of a simple ferromagnetic material as well. The drawback to the mean field approach is that one must *assume* that all atoms must all act the same. The problem becomes more tractable when the agents are only allowed to interact with their nearest neighbors and can be in only two possible states. The easiest case being an Ising model. The purpose of this paper is to illustrate the use of the ME method as an approximation tool. The paper show a simple case to compare with the traditional mean field approach. Then we show two examples that lie outside of traditional methodologies. These cases explore a ferromagnetic material with *defects*. The main result is that regardless of the case, the ME method provides good approximations for each case which would not otherwise be possible or at least well justified.

1 Introduction

In a simple ferromagnetic material (single domain), the electronic spin of the individual atoms are strong enough to affect one and other, the so called "exchange" interaction [1]. However this effect is temperture dependent. When the temperture is below a certain point (the Curie temperture) the spins tend to all point in the same direction due to their influence on each other. This establishes a permanant magnet as the individuals produce a net dipole effect. Above this temperture, the atoms cease to have a significant effect on each other and the material behaves more like a paramagnetic substance. Determining this net dipole effect can be difficult. First, the interactions are due to complicated quantum effects. Second, since a given material as a very large number of atoms, computing the net dipole effect can be difficult in two dimensions and completely intractable in three dimensions. Therefore approximations are made to facilitate computational difficulties such as using an Ising Model and or the mean field approximation.

In 1957, Jaynes [2] showed that maximizing statistical mechanic entropy for the purpose of revealing how gas molecules were distributed was simply the maximizing of Shannon's information entropy [3] with statistical mechanical information. This idea lead to MaxEnt or his use of the Method of Maximum Entropy for assigning probabilities. This method has evolved to a more general method, the method of Maximum (relative) Entropy (ME) [4] which has the advantage of not only assigning probabilities but *updating* them when new information is given in the form of constraints on the family of allowed posteriors. One of the drawbacks of the MaxEnt method was the inability to include data. When data was present, one used Bayesian methods. The methods were combined in such a way that MaxEnt was used for assigning a prior for Bayesian methods, as Bayesian methods could not deal with information in the form of constraints, such as expected values.

Previously it has been shown that one can use ME to reproduce a mean field solution for a simple fluid [5]. The purpose of this was to illustrate that in addition to updating probabilities, ME can also be used as an approximation tool. The purpose of our paper is to illustrate the use of the ME method as a tool for attaining approximations for ferromagnetic materials that lie outside the ability of traditional methods. In doing so we further the the previous work done and show the versitility of the method.

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In the second section of this paper we show the traditional methods for attaining an approximation, the Ising model and the mean field field approximation. The third section shows how ME can not only reproduce the mean field approximation, but does so using fewer assumptions. In the fourth section we provide two examples that lie outside the capabilities of traditional methodologies. These cases explore a ferromagnetic material with *defects*. The main result is that regardless of the case, the ME method provides good approximations for each case which would not otherwise be possible or at least well justified.

2 The Ising model and the mean field approximation

The drawback to the mean field approach is that one must *assume* that all atoms must all act the same. Additionally, the problem is only tractable when the atoms are only allowed to interact with their nearest neighbors and assumed to be in only two possible states. This model is called the Ising model.

2.1 The Ising Model

Although these exchange interactions are quantum related, Ernst Ising [6] suggested that one should examine a simple model where the atomic spins are related by simple spins of +1 and -1 or spin "up" and spin "down". Further, he suggested to neglect all exchange interactions *except* those between nearest neighbors. Using these two assumptions, the exchange interaction energy can be calculated as follows:

$$H = -J \sum_{i,j}^{N,n} s_i s_j , \quad (1)$$

where N is the number of atoms, J is the exchange interaction energy and s is the net electronic spin of the atom where $s = \{+1, -1\}$. The standard partition function for this system would then be written as,

$$Z = \sum_{\{s_i\}} e^{-\beta H} , \quad (2)$$

where $\sum_{\{s_i\}} = \sum_{s_1} \sum_{s_2} \dots \sum_{s_N}$ and β is usual thermodynamic value $1/kT$ where T is the temperature and k is the Boltzmann constant. For the one dimensional case, the partition function can easily be calculated,

$$Z = 2^N (\cosh \beta J)^{N-1} \approx (2 \cosh \beta J)^N \text{ (for large } N\text{).} \quad (3)$$

The resulting average energy would then be,

$$\bar{H} = -\frac{\partial \ln Z}{\partial \beta} = -N J \tanh \beta J . \quad (4)$$

2.2 The mean field approximation

Although the Ising model's partition function can be solved exactly, this is only true for one dimension. It fails for real ferromagnetic substances since it only takes into account two near neighbors. For three dimensional materials, each atom may have 6, 8 or even 12 close neighbors depending on the crystal geometry. This is where another approximation is made and it is commonly referred to as the mean field approximation [1, 6].

We start with the same energy function as above (1) but now examine only one atom (sometimes called the "central" atom),

$$H_i = -J s_i \sum_{,j}^n s_j . \quad (5)$$

Where H_i is the energy for one atom and n is the number of nearest neighbors (ex. a face-centered cubic lattice would have 12) with atoms at the edge of the material neglected. Now we assume that each neighbor contributes equally and *average* over the neighbor spins around this one atom,

$$\bar{H}_i = -J s_i n \bar{s}_j , \quad (6)$$

where $\bar{s}_i = \sum_{,j}^n \frac{s_j}{n}$ and the Boltzmann probability for finding this atom in the s_i state is

$$p_i = \frac{1}{Z_i} e^{-\beta H_i} , \quad (7)$$

where $Z_i = 2 \cosh \beta J n \bar{s}_j$. Now we take the average of for this one atom over its two possible states,

$$\langle s_i \rangle = \sum_{s_i} s_i p_i = \frac{1}{Z_i} [(1)e^{\beta H_i} + (-1)e^{-\beta H_i}] = \frac{2 \sinh \beta J n \bar{s}_j}{2 \cosh \beta J n \bar{s}_j} = \tanh \beta J n \bar{s}_j . \quad (8)$$

The next assumption is that all of the *all* atoms will behave like this one. Therefore, the average spin for the entire material is

$$\bar{s} = \langle \langle s_i \rangle \rangle = \langle \bar{s}_j \rangle , \quad (9)$$

which now allows us to write

$$\bar{s} = \tanh \beta J n \bar{s} , \quad (10)$$

which is the final result for this section. This equation can then be used to solve for the Curie temperature, the total magnetic moment and the magnetic susceptibility. To be more general, an external magnetic field can be applied as well which would alter the solution but not the form. For this case, the Hamiltonian would be,

$$\bar{H}_{i\text{eff}} = -J s_i n \bar{s}_j - \mu B s_i = -\epsilon s_i , \quad (11)$$

where μ is the magnetic moment, B is the magnetic field strength and ϵ is the net effective energy on the i^{th} atom. Note however that while this does not alter the solution using the mean field approximation because this is the effective Hamiltonian (11) for a single atom. In other words, the averaging is already taken into account in the effective Hamiltonian. If one were to write the full Hamiltonian with the external field instead of (1) above, then one will not have as simple of a solution for (3), i.e. $Z_{\text{eff}} \neq (2 \cosh \beta \epsilon)^N$.

3 Using ME for the approximation

Part of the strength of using ME is that one does not need to justify some of the *assumptions* such as those used above (4 explicitly used, many hidden). One simply supplies the information that one has available and allows the method to turn out the most honest solution based on the information given. This can be demonstrated by using the method to find an appropriate approximation for a ferromagnetic material given the information that one has available. We show in this section where ME was used for this very same task to arrive at a similar solution as above.

We start by writing the full posterior solution for a ferromagnetic *system* (all atoms) which is a canonical distribution,

$$p\{s\} = \frac{1}{Z} e^{-\beta H\{s\}} , \quad (12)$$

where $p\{s\} = p(s_1 \dots s_N)$, Z is the partition function from (2) with $H\{s\}$ being some general Hamiltonian and N the number of atoms. NOTE: This function can be ascertained by using the ME method without assumptions as Jaynes did for Gibbs' canonical function when he used his special case of ME, MaxEnt [2]. However, to determine the values of the Curie temperature, the total magnetic moment and the magnetic susceptibility we are faced with the same dilemma as above; we cannot compute the solutions exactly. Therefore, we must try to find an approximation that is tractable. For *illustrative* purposes, we will adopt the Ising model so as to show how one can use ME to arrive at a similar approximation as the mean field produces. For this we let

$$H\{s\} = H_{\text{int}} + H_{\text{ext}} = -J \sum_{i,j}^{N,n} s_i s_j - \sum_i^N \mu B s_i , \quad (13)$$

where in $H_{\text{int}} = H$ from (1) and H_{ext} is the energy due to external magnetic field acting on the atoms. We now wish to use ME to find an approximation that is tractable. We accomplish this by first writing down the appropriate entropy,

$$S[p_A|p] = - \sum_{\{s\}} p_A \log \frac{p_A}{p} , \quad (14)$$

where p is the canonical probability using (13) and p_A is the approximation that we seek. We proceed rewriting the entropy as

$$S[p_A|p] = - \sum_{\{s\}} p_A \log p_A + \sum_{\{s\}} p_A \log p , \quad (15)$$

or substituting with the canonical form for p , (12)

$$S[p_A|p] = \frac{1}{k}S_A - \sum_{\{s\}} p_A \beta H\{s\} - \beta F, \quad (16)$$

where Z can also be written as $Z = e^{-\beta F}$ where F is the free energy. This can further be reduced to

$$S[p_A|p] = \frac{1}{k}S_A + \beta(F - \langle H\{s\} \rangle_A), \quad (17)$$

where $\langle H\{s\} \rangle_A = \sum_{\{s\}} p_A H\{s\}$ which can also be seen as the energy E_A of the system. Since by definition, $S[p_A|p] \leq 0$ we can write,

$$F \leq E_A - TS_A. \quad (18)$$

When using the ME method, we maximize the entropy to find the best posterior given the information provided. For this specific case, we have rewritten the entropy form in terms of an inequality that compares the free energy of the system, F with the approximate values for the average energy, E_A and the entropy S_A . The free energy is minimized to determine the best approximation for F , which is called the Bogoliubov Variational Principle.[5]. However, this is simply a special case of ME. To be more general, we proceed with using the ME method to find the best approximation.

When using the ME method, the goal is to search the family of possible posteriors to find the one that maximizes the entropy given the constraints. In addition to this, we all need a solution that is trackable. Therefore, we seek a posterior that has a form,

$$p_A = \frac{1}{Z_A} e^{-\beta H_A}, \quad (19)$$

where $H_A = -\sum_i \epsilon_{iA} s_i$ and ϵ_{iA} is some *effective* energy similar to (11). Again for illustrative purposes we assume that all atoms poses the same effective energy so that $\epsilon_{iA} = \epsilon_A$. The difference is that we do not yet *know* the form of ϵ_A . We continue by following a similar route to (8) by writing the expectation value for s_i with respect to p_A ,

$$\langle s_i \rangle_A = \sum_{\{s_i\}} s_i p_A = \tanh \beta \epsilon_{iA} = \tanh \beta \epsilon_A, \quad (20)$$

Except that here we are *marginalizing* over all atoms except the i^{th} . Notice that because ϵ_A is constant, the solution is independent of i . Next we maximize (14) or in keeping with the current case, we minimize the free energy, F . Rewriting (18)

$$\beta F_{\min} = -\frac{1}{k}S_A + \beta \langle H\{s\} \rangle_A \quad (21)$$

Substituting in (19) and rewriting,

$$F_{\min} = \left(\frac{1}{\beta} \sum_{\{s\}} p_A \log e^{-\beta H_A} - \frac{1}{\beta} \sum_{\{s\}} p_A \log Z_A \right) + \sum_{\{s\}} p_A H\{s\}, \quad (22)$$

as Z_A is a constant it can be pulled out of the summation and since $\sum_{\{s\}} p_A = 1$,

$$F_{\min} = \left(-\frac{1}{\beta} \sum_{\{s\}} p_A \beta H_A - \frac{1}{\beta} \log Z_A \right) + \sum_{\{s\}} p_A H\{s\} \quad (23)$$

or

$$F_{\min} = -\langle H_A \rangle_A - \frac{1}{\beta} \log Z_A + \langle H\{s\} \rangle_A. \quad (24)$$

We now substitute our Hamiltonians into the function,

$$F_{\min} = - \left\langle -\epsilon_A \sum_i s_i \right\rangle_A - \frac{1}{\beta} \log Z_A + \left\langle -J \sum_{i,j}^{N,n} s_i s_j - \sum_i^N \mu B s_i \right\rangle_A, \quad (25)$$

and substituting $\langle \sum_i s_i \rangle_A = \sum_i \langle s_i \rangle_A = N \langle s_i \rangle_A = N \tanh \beta \epsilon_A$ yields,

$$F_{\min} = \epsilon_A N \tanh \beta \epsilon_A - \frac{1}{\beta} \log Z_A - J \sum_{i,j}^{N,n} \langle s_i s_j \rangle_A - \mu B N \tanh \beta \epsilon_A . \quad (26)$$

Then substituting $Z_A \approx (2 \cosh \beta \epsilon_A)^N$ yields,

$$F_{\min} = \epsilon_A N \tanh \beta \epsilon_A - \frac{1}{\beta} \log(2 \cosh \beta \epsilon_A)^N - J \sum_{i,j}^{N,n} \langle s_i s_j \rangle_A - \mu B N \tanh \beta \epsilon_A \quad (27)$$

and since (20) is independent of i , $\langle s_i \rangle_A = \langle s_j \rangle_A$ and $\langle s_i s_j \rangle_A = \langle s_i \rangle_A \langle s_j \rangle_A$, we can write,

$$F_{\min} = \epsilon_A N \tanh \beta \epsilon_A - \frac{1}{\beta} N \log(2 \cosh \beta \epsilon_A) - J \sum_{i,j}^{N,n} \langle s_i \rangle_A \langle s_j \rangle_A - \mu B N \tanh \beta \epsilon_A . \quad (28)$$

Substituting (20) into the equation yields,

$$F_{\min} = \epsilon_A N \tanh \beta \epsilon_A - \frac{N}{\beta} \log(2 \cosh \beta \epsilon_A) - J \frac{1}{2} N n (\tanh \beta \epsilon_A)^2 - \mu B N \tanh \beta \epsilon_A , \quad (29)$$

where the factor n comes from the number of nearest neighbors, the factor N is from the total number of atoms and the $1/2$ is due to double counting.

Now we choose the form that minimizes F_{\min} with respect to ϵ_A ,

$$\begin{aligned} \frac{\partial F_{\min}}{\partial \epsilon_A} &= 0 = N \tanh \beta \epsilon_A + N \epsilon_A \frac{\beta}{\cosh^2 \beta \epsilon_A} - \frac{N}{\beta} \frac{\beta \sinh \beta \epsilon_A}{\cosh \beta \epsilon_A} \\ &\quad - J \frac{1}{2} N n 2 \tanh \beta \epsilon_A \frac{\beta}{\cosh^2 \beta \epsilon_A} - \mu B N \frac{\beta}{\cosh^2 \beta \epsilon_A} , \end{aligned} \quad (30)$$

or rewritten,

$$\begin{aligned} 0 &= N \tanh \beta \epsilon_A + N \epsilon_A \frac{\beta}{\cosh^2 \beta \epsilon_A} - N \tanh \beta \epsilon_A \\ &\quad - J N n \tanh \beta \epsilon_A \frac{\beta}{\cosh^2 \beta \epsilon_A} - \mu B N \frac{\beta}{\cosh^2 \beta \epsilon_A} . \end{aligned} \quad (31)$$

After canceling terms we have,

$$0 = \epsilon_A - \mu B - J n \tanh \beta \epsilon_A \quad (32)$$

or better,

$$\epsilon_A - \mu B = J n \tanh \beta \epsilon_A . \quad (33)$$

This is our final result for this section. Notice that if $B = 0$ then we recover our solution using the mean field approximation above. If we let $\epsilon_A = J n \bar{s}$ we rewrite the above equation,

$$J n \bar{s} = J n \tanh \beta J n \bar{s} , \quad (34)$$

and after cancelations,

$$\bar{s} = \tanh \beta J n \bar{s} . \quad (35)$$

which is (10).

However, from (33) *alone* we can solve for the Curie temperature, the total magnetic moment and the magnetic susceptibility in the usual way [7]. This is true even though we still do not *know* the form for ϵ_A . Using this approach, we did not need to assume that all atoms behave like a "central" atom and we did not need to know the explicit form of the effective energy, only that there was one. Following the ME method we simply processed all of our information that we had available. Notice that we also no longer need to *assume* Ising conditions. We explore such possible scenarios in the next section.

4 The defective Ising model

4.1 Three state example

In the Ising model, the possible states are spin up and spin down. Let us examine the case where there are *three* possible states. In this example, we will let $s = \{+1, 0, -1\}$ where an atom in the zero, 0 state would contribute no energy, like perhaps a defect of some kind. We proceed with the method above up until (20) where the the new expected value for a particular atom for this case would be,

$$\langle s_i \rangle_A = \sum_{\{s_i\}} s_i p_A = \frac{2 \sinh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} . \quad (36)$$

Continuing the steps above, we write our new F_{\min} ,

$$F_{\min} = \epsilon_A N \frac{2 \sinh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} - \frac{N}{\beta} \log(2 \cosh \beta \epsilon_A + 1) - J \frac{1}{2} N n \left(\frac{2 \sinh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} \right)^2 - \mu B N \frac{2 \sinh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} , \quad (37)$$

and minimize this function once again with respect to ϵ_A which yields,

$$\begin{aligned} \frac{\partial F_{\min}}{\partial \epsilon_A} = 0 = & N \frac{2 \sinh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} + N \epsilon_A \left(\frac{\beta 2 \cosh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} - \frac{\beta 4 \sinh^2 \beta \epsilon_A}{(2 \cosh \beta \epsilon_A + 1)^2} \right) - \frac{N}{\beta} \frac{2 \beta \sinh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} \\ & - J \frac{1}{2} N n 2 \left(\frac{2 \sinh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} \right) \left(\frac{\beta 2 \cosh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} - \frac{\beta 4 \sinh^2 \beta \epsilon_A}{(2 \cosh \beta \epsilon_A + 1)^2} \right) - \mu B N \left(\frac{\beta 2 \cosh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} - \frac{\beta 4 \sinh^2 \beta \epsilon_A}{(2 \cosh \beta \epsilon_A + 1)^2} \right) \end{aligned}$$

After canceling terms we arrive at,

$$\epsilon_A - \mu B = J n \left(\frac{2 \sinh \beta \epsilon_A}{2 \cosh \beta \epsilon_A + 1} \right) . \quad (40)$$

Which is our final result. This equation can then be used as above to solve for the Curie temperature, the total magnetic moment and the magnetic susceptibility for this material.

To make this result a little more general we can also write,

$$\epsilon_A - \mu B = J n_G \left(-\frac{\partial \ln Z_A}{\partial \epsilon_A} \right) = J n_G \beta \left(\frac{\partial F_A}{\partial \epsilon_A} \right) = J n_G (\langle s_i \rangle_A) , \quad (41)$$

where Z_A is once again the *approximate* partition function, n_G are the nearest neighbors and F_A is the *approximate* free energy.

4.2 Two energy example

In the previous example, we examined a three state atom. In this example, we examine a material that has an *known* defect. Perhaps the material was scanned in some way and a defect was found. In this case, we need to use *two* effective energy terms. One for the atoms that are surrounded by non-defective atoms, ϵ_{ND} and one for the ones affected by the defect, ϵ_D . For illustrative purposes, we will examine the case where we have one defective atom. This means that there are $N - n - 1$ atoms that are surrounded by non-defective atoms, n atoms that have one defective atom next to it and 1 atom which is the defective atom. For our purposes, let's think of the defect as an empty slot. Therefore, the actual Hamiltonian would be,

$$H \{s\} = H_{int} + H_{ext} = -J \sum_{i,j}^{N-n-1, n} s_i s_j - J \sum_{k,l}^{n, n-1} s_k s_l - J s_0 - \sum_i^{N-n-1} \mu B s_i - \sum_k^n \mu B s_k - \mu B s_0 ,$$

where i are the non-defective atoms, j are neighbors (n) for these atoms, k are the atoms affected by the defect, l are the neighbors ($n - 1$) of the affected atoms and s_0 is the defective atom. Since we are looking at this as an empty slot, we let $s_0 = 0$. Now we write our estimated Hamiltonian for this case,

$$H_A = -\epsilon_{ND} \sum_i s_i - \epsilon_D \sum_k s_k .$$

Following the same procedures above, we attain *two* expected values, one for each effective energy,

$$\langle s_i \rangle_A = \sum_{\{s_i\}} s_i p_A = \tanh \beta \epsilon_{ND} \quad (42)$$

and

$$\langle s_k \rangle_A = \sum_{\{s_i\}} s_k p_A = \tanh \beta \epsilon_D . \quad (43)$$

Once again we write down the function we wish to minimize,

$$F_{\min} = -\langle H_A \rangle_A - \frac{1}{\beta} \log Z_A + \langle H \{s\} \rangle_A , \quad (44)$$

and substituting in our Hamiltonians yields,

$$F_{\min} = - \left\langle -\epsilon_{ND} \sum_i^{N-n-1} s_i - \epsilon_D \sum_k^n s_k \right\rangle_A - \frac{1}{\beta} \log Z_A + \left\langle -J \sum_{i,j}^{N-n-1, n} s_i s_j - J \sum_{k,l}^{n, n-1} s_k s_l - \sum_i^{N-n-1} \mu B s_i - \sum_k^n \mu B s_k \right\rangle_A . \quad (45)$$

Substituting $\langle \sum_i s_i \rangle_A = \sum_i \langle s_i \rangle_A = (N - n - 1) \langle s_i \rangle_A = (N - n - 1) \tanh \beta \epsilon_{ND}$ and $\langle \sum_k s_k \rangle_A = \sum_k \langle s_k \rangle_A = n \langle s_k \rangle_A = n \tanh \beta \epsilon_D$ yields,

$$F_{\min} = \epsilon_{ND} (N - n - 1) \tanh \beta \epsilon_{ND} + \epsilon_D n \tanh \beta \epsilon_D - \frac{1}{\beta} \log (Z_{ND} Z_D) \quad (46)$$

$$-J \sum_{i,j}^{N-n-1, n} \langle s_i s_j \rangle_{ND} - J \sum_{k,l}^{n, n-1} \langle s_k s_l \rangle_D - \mu B [\epsilon_{ND} (N - n - 1) \tanh \beta \epsilon_{ND} + \epsilon_D n \tanh \beta \epsilon_D] \quad (47)$$

where $Z_A = Z_{ND} Z_D$. Substituting $Z_{ND} \approx (2 \cosh \beta \epsilon_{ND})^{(N-n-1)}$ and $Z_D \approx (2 \cosh \beta \epsilon_D)^{(n)}$ yields,

$$F_{\min} = \epsilon_{ND} (N - n - 1) \tanh \beta \epsilon_{ND} + \epsilon_D n \tanh \beta \epsilon_D - \frac{1}{\beta} \log (2 \cosh \beta \epsilon_{ND})^{N-n-1} - \frac{1}{\beta} \log (2 \cosh \beta \epsilon_D)^n \quad (48)$$

$$-J \sum_{i,j}^{N-n-1, n} \langle s_i s_j \rangle_{ND} - J \sum_{k,l}^{n, n-1} \langle s_k s_l \rangle_D - \mu B [\epsilon_{ND} (N - n - 1) \tanh \beta \epsilon_{ND} + \epsilon_D n \tanh \beta \epsilon_D] . \quad (49)$$

Since (42) and (43) are independent of i and k respectively, $\langle s_i \rangle_A = \langle s_j \rangle_A$ and $\langle s_i s_j \rangle_A = \langle s_i \rangle_A \langle s_j \rangle_A$, we can write,

$$F_{\min} = \epsilon_{ND} (N - n - 1) \tanh \beta \epsilon_{ND} + \epsilon_D n \tanh \beta \epsilon_D - \frac{1}{\beta} \log (2 \cosh \beta \epsilon_{ND})^{N-n-1} - \frac{1}{\beta} \log (2 \cosh \beta \epsilon_D)^n \quad (50)$$

$$-J \sum_{i,j}^{N-n-1, n} \langle s_i \rangle_{ND} \langle s_j \rangle_{ND} - J \sum_{k,l}^{n, n-1} \langle s_k \rangle_D \langle s_l \rangle_D - \mu B [\epsilon_{ND} (N - n - 1) \tanh \beta \epsilon_{ND} + \epsilon_D n \tanh \beta \epsilon_D] \quad (51)$$

Substituting (42) and (43) into the equation yields,

$$F_{\min} = \epsilon_{ND} (N - n - 1) \tanh \beta \epsilon_{ND} + \epsilon_D n \tanh \beta \epsilon_D - \frac{1}{\beta} \log (2 \cosh \beta \epsilon_{ND})^{N-n-1} - \frac{1}{\beta} \log (2 \cosh \beta \epsilon_D)^n \quad (52)$$

$$- \frac{1}{2} J (N - n - 1) n \tanh^2 \beta \epsilon_{ND} - \frac{1}{2} J (n) (n - 1) \tanh^2 \beta \epsilon_D - \mu B [\epsilon_{ND} (N - n - 1) \tanh \beta \epsilon_{ND} + \epsilon_D n \tanh \beta \epsilon_D] \quad (53)$$

and after collecting ϵ_{ND} and ϵ_D like terms we have,

$$F_{\min} = \epsilon_{ND} (N - n - 1) \tanh \beta \epsilon_{ND} - \frac{1}{\beta} \log (2 \cosh \beta \epsilon_{ND})^{N-n-1} - \frac{1}{2} J (N - n - 1) n \tanh^2 \beta \epsilon_{ND} \mu B \epsilon_{ND} (N - n - 1) \tanh \beta \epsilon_D - \epsilon_D n \tanh \beta \epsilon_D - \frac{1}{\beta} \log (2 \cosh \beta \epsilon_D)^n - \frac{1}{2} J (n) (n - 1) \tanh^2 \beta \epsilon_D + \mu B \epsilon_D n \tanh \beta \epsilon_D ,$$

where the factor n comes from the number of nearest neighbors, the factor N is from the total number of atoms and the $1/2$ is due to double counting.

Now we choose the form that minimizes F_{\min} with respect to ϵ_{ND} and ϵ_{D} ,

$$\begin{aligned} \frac{\partial F_{\min}}{\partial \epsilon_{\text{ND}}} &= 0 = (N - n - 1) \tanh \beta \epsilon_{\text{ND}} + (N - n - 1) \epsilon_{\text{ND}} \frac{\beta}{\cosh^2 \beta \epsilon_{\text{ND}}} - \frac{N - n - 1}{\beta} \frac{\beta \sinh \beta \epsilon_{\text{ND}}}{\cosh \beta \epsilon_{\text{ND}}} \\ &\quad - J \frac{1}{2} (N - n - 1) (n) 2 \tanh \beta \epsilon_{\text{ND}} \frac{\beta}{\cosh^2 \beta \epsilon_{\text{ND}}} - \mu B (N - n - 1) \frac{\beta}{\cosh^2 \beta \epsilon_{\text{ND}}} \end{aligned} \quad (54)$$

$$\begin{aligned} 0 &= (N - n - 1) \tanh \beta \epsilon_{\text{ND}} + (N - n - 1) \epsilon_{\text{ND}} \frac{\beta}{\cosh^2 \beta \epsilon_{\text{ND}}} - \frac{N - n - 1}{\beta} \frac{\beta \sinh \beta \epsilon_{\text{ND}}}{\cosh \beta \epsilon_{\text{ND}}} \\ &\quad - J (N - n - 1) (n) \tanh \beta \epsilon_{\text{ND}} \frac{\beta}{\cosh^2 \beta \epsilon_{\text{ND}}} - \mu B (N - n - 1) \frac{\beta}{\cosh^2 \beta \epsilon_{\text{ND}}} \end{aligned} \quad (55)$$

$$\begin{aligned} 0 &= \epsilon_{\text{ND}} - J (n) \tanh \beta \epsilon_{\text{ND}} - \mu B \\ \epsilon_{\text{ND}} - \mu B &= J n \tanh \beta \epsilon_{\text{ND}} \\ \epsilon_{\text{D}} - \mu B &= J (n - 1) \tanh \beta \epsilon_{\text{D}} \end{aligned} \quad (56)$$

Which is our final result. These equations can then be used as above to solve for the Curie temperature, the total magnetic moment and the magnetic susceptibility for this material as usual. The difference here is that we will have two of each. For example, a Curie temperature that applies to most of the atoms, and one that is local to the defect. Therefore, the total magnetic moment will not simple be a result of just one temperature but a sum of each magnetic moment determined by the equations. Notice that (41) still holds in general. In the two energy case, for one energy the number of nearest neighbors, $n_G = n$ and for the second energy, $n_G = n - 1$.

5 Conclusions

We described the traditional Ising model of a ferromagnetic material and the mean field approximation for a multidimensional material. It has been shown that not only can the Me method be used for updateing, but for determining approximations as well.

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References

- [1] F. Reif, *Fundamentals of Statistical and Thermal Physics*, (McGraw-Hill 1965).
- [2] E. T. Jaynes, Phys. Rev. **106**, 620 and **108**, 171 (1957).
- [3] C. E. Shannon, "A Mathematical Theory of Communication", *Bell System Technical Journal*, **27**, 379, (1948).
- [4] A. Caticha and A. Giffin, "Updating Probabilities", *Bayesian Inference and Maximum Entropy Methods in Science and Engineering*, ed. A. Mohammad-Djafari, AIP Conf. Proc. **872**, 31 (2006) (<http://arxiv.org/abs/physics/0608185>).
- [5] C.Y. Tseng, "The Maximum Entropy Method in Statistical Physics: an Alternative Approach to the Theory of Simple Fluids", Ph. D. Thesis, SUNY at Albany, Albany, 2004 (New York- USA).
- [6] D. V. Schroeder, *An Introduction to Thermal Physics*, (Addison Wesley Longman 2000).
- [7] A. Caticha, Class notes on "Principles of Information Physics", (Univ at Albany - SUNY, 2007).